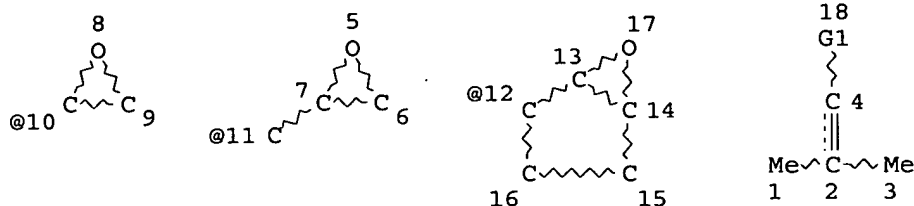


=> d que 122

L5 311 SEA FILE=HCAPLUS ABB=ON PLU=ON "POLYMERIZATION CATALYSTS (L)
LEWIS ACID"+PFT/CT
L6 5455 SEA FILE=HCAPLUS ABB=ON PLU=ON LEWIS ACIDS+NT/CT
L14 STR



VAR G1=11/10/12

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L16 965 SEA FILE=REGISTRY SSS FUL L14

L17 107 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 (L) (RACT OR RGT OR RCT)/RL

L18 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L17 AND (L5 OR L6 OR LEWIS)

L21 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L17 AND ?LUMIN?

L22 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 OR L21

=> d 122 ibib abs hitind hitstr 1-4

L22 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:751588 HCAPLUS

DOCUMENT NUMBER: 141:379730

TITLE: Towards a total synthesis of quinocarcin:

Diastereoselective synthesis of functionalized
azepino[1,2-b]isoquinolinesAUTHOR(S): Koepler, Oliver; Laschat, Sabine; Baro, Angelika;
Fischer, Peter; Miehl, Burkhard; Hotfilder, Marc;
le Viseur, ChristophCORPORATE SOURCE: Institut fuer Organische Chemie der Technischen
Universitaet Braunschweig, Braunschweig, 38106,
GermanySOURCE: European Journal of Organic Chemistry (2004), (17),
3611-3622

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

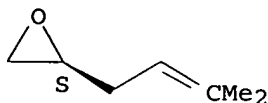
LANGUAGE: English

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

- AB 1,3-Disubstituted tetrahydro-oxazolo-isoquinolinones I (R = α -CO₂Et or β -CO₂Et) were obtained from phenylalanine in seven steps and 42% overall yield by Katritzky's benzotriazole method. The tricyclic oxazolidinone I (R = α -CO₂Et) was further converted into amino alc. II (R = α -CH₂OMe) by employing a chemoselective reduction of the ester group with LiBH₄/MeOH. Compound II (R = α -CH₂OMe) and the corresponding 1-unsubstituted tetrahydroisoquinoline alc. II (R = H) were converted into aldehydes III and IV, which cyclized in the presence of different **Lewis** acids to give the substituted azepino[1,2-b]isoquinolines V and VI, resp., which are key structural features of the alkaloid quinocarcin (VII). The stereoselectivities of the **Lewis**-acid-catalyzed heteroene reaction are highly dependent on the substitution pattern and the type of **Lewis** acid.
- CC 26-6 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 27
- ST asym synthesis azepinoisoquinoline **Lewis** acid catalyzed heteroene cyclization quinocarcin; antitumor agent human Ewing's sarcoma azepinoisoquinoline quinocarcin
- IT Cyclization catalysts
(**Lewis** acid-catalyzed hetero-ene cyclization catalysts; diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)
- IT Addition reaction catalysts
(ene, **Lewis** acid-catalyzed hetero-ene cyclization catalysts; diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)
- IT Addition reaction
(ene, stereoselective, **Lewis** acid-catalyzed hetero-ene cyclization; diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)
- IT Cyclization
(stereoselective, **Lewis** acid-catalyzed hetero-ene cyclization; diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)
- IT 2510-33-0P 215928-81-7P 219640-74-1P 223460-44-4P 782500-81-6P
782500-84-9P 782500-85-0P 782500-86-1P 782500-87-2P
782500-89-4P 782500-90-7P 782500-91-8P 782500-92-9P
782500-93-0P 782500-95-2P 782500-96-3P 782500-97-4P 782501-01-3P
782501-02-4P 782501-04-6P
RL: **RCT** (**Reactant**); SPN (Synthetic preparation); PREP (Preparation); **RACT** (**Reactant or reagent**)
(diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)
- IT 109-63-7 563-43-9, **Ethylaluminum** dichloride, reactions
7550-45-0, Titanium tetrachloride, reactions 7646-78-8, Tin tetrachloride, reactions 7646-85-7, Zinc (II) chloride, reactions
RL: RGT (**Reagent**); **RACT** (**Reactant or reagent**)
(diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)
- IT **782500-89-4P**
RL: **RCT** (**Reactant**); SPN (Synthetic preparation); PREP (Preparation); **RACT** (**Reactant or reagent**)
(diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)
- RN 782500-89-4 HCAPLUS
- CN Oxirane, (3-methyl-2-butenyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:385564 HCAPLUS

DOCUMENT NUMBER: 139:117351

TITLE: Biomimetic Synthesis of Fused Polypyrans:
Oxacyclization Stereo- and Regioselectivity Is a
Function of the Nucleophile

AUTHOR(S): Bravo, Fernando; McDonald, Frank E.; Neiwert, Wade A.;
Do, Bao; Hardcastle, Kenneth I.

CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta,
GA, 30322, USA

SOURCE: Organic Letters (2003), 5(12), 2123-2126

CODEN: ORLEF7; ISSN: 1523-7060

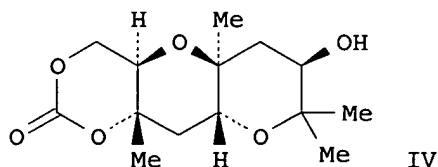
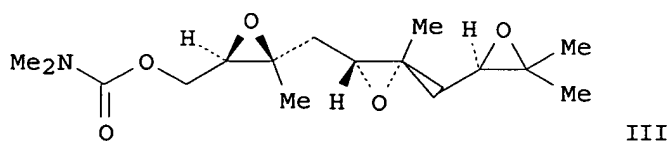
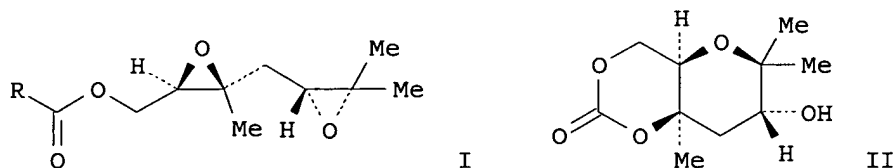
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:117351

GI



AB The stereoselectivity of **Lewis** acid-induced endo-regioselective oxacyclizations of 1,4-diepoxides is dependent upon the nature of the terminating nucleophile. For instance, ring-opening/recyclization of the carbonate-substituted diepoxide I (R = Me₃CO) provides a cis-fused bicyclic product II, whereas carbamate-derived I (R = Me₂N) affords the

trans-fused diastereomer of II. Stereospecific and regioselective conversion of the tertiary carbamate-terminated 1,4,7-triepoxyde III to tricyclic all-trans-fused polypyran IV is also demonstrated.

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 565183-88-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(allylic oxidation; biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

IT 565183-76-8P 565183-77-9P 565183-78-0P 565183-80-4P 565183-82-6P

565183-84-8P 565183-90-6P 565183-91-7P 565183-92-8P

565183-93-9P 565183-94-0P 565183-95-1P 565183-96-2P

565183-98-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

IT 43161-23-5P 565183-74-6P 565183-79-1P

565183-81-5P 565183-83-7P 565183-89-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(epoxidn.; biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

IT 565183-88-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

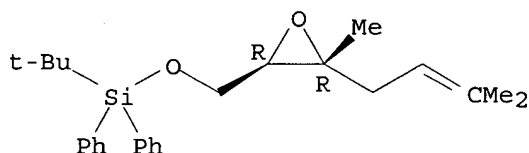
(Preparation); RACT (Reactant or reagent)

(allylic oxidation; biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

RN 565183-88-2 HCAPLUS

CN Silane, (1,1-dimethylethyl) [[(2R,3R) -3-methyl-3-(3-methyl-2-butenyl)oxiranyl]methoxy]diphenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 565183-92-8P 565183-93-9P 565183-94-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

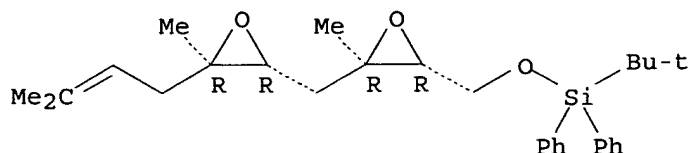
(Preparation); RACT (Reactant or reagent)

(biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

RN 565183-92-8 HCAPLUS

CN L-glucio-Heptitol, 2,3:5,6-dianhydro-4,7-dideoxy-1-O-[(1,1-dimethylethyl)diphenylsilyl]-3-C-methyl-6-C-(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)

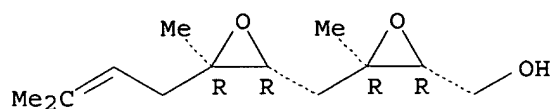
Absolute stereochemistry.



RN 565183-93-9 HCAPLUS

CN L-glucitol, 2,3:5,6-dianhydro-4,7-dideoxy-3-C-methyl-6-C-(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)

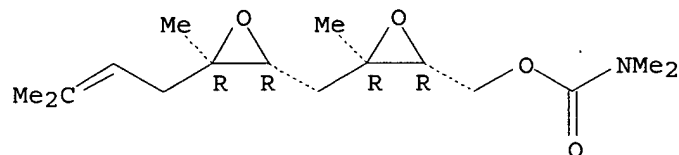
Absolute stereochemistry. Rotation (+).



RN 565183-94-0 HCAPLUS

CN L-glucitol, 2,3:5,6-dianhydro-4,7-dideoxy-3-C-methyl-6-C-(3-methyl-2-butenyl)-, dimethylcarbamate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 565183-74-6P 565183-79-1P 565183-81-5P

565183-83-7P

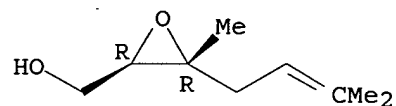
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(epoxidn.; biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

RN 565183-74-6 HCAPLUS

CN Oxiranemethanol, 3-methyl-3-(3-methyl-2-butenyl)-, (2R,3R)- (9CI) (CA INDEX NAME)

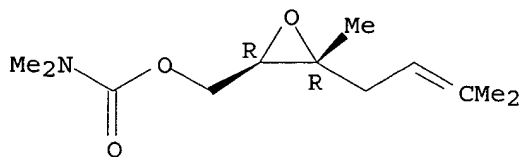
Absolute stereochemistry. Rotation (+).



RN 565183-79-1 HCAPLUS

CN Carbamic acid, dimethyl-, [(2R,3R)-3-methyl-3-(3-methyl-2-butenyl)oxiranyl]methyl ester (9CI) (CA INDEX NAME)

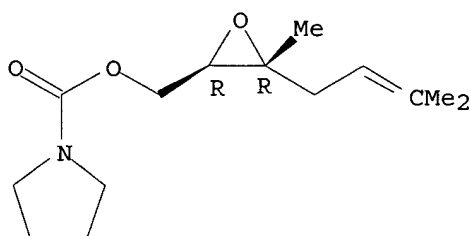
Absolute stereochemistry. Rotation (+).



RN 565183-81-5 HCAPLUS

CN 1-Pyrrolidinecarboxylic acid, [(2R,3R)-3-methyl-3-(3-methyl-2-butenyl)oxiranyl]methyl ester (9CI) (CA INDEX NAME)

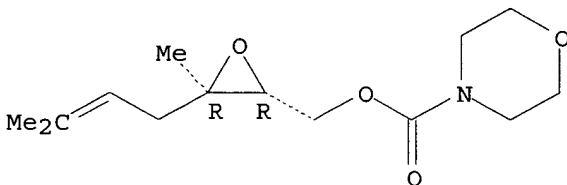
Absolute stereochemistry.



RN 565183-83-7 HCAPLUS

CN 4-Morpholinecarboxylic acid, [(2R,3R)-3-methyl-3-(3-methyl-2-butenyl)oxiranyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:538472 HCAPLUS

DOCUMENT NUMBER: 119:138472

TITLE: A tellurium transposition route to allylic alcohols: overcoming some limitations of the Sharpless-Katsuki asymmetric epoxidation

AUTHOR(S): Dittmer, Donald C.; Discordia, Robert P.; Zhang, Yanzhi; Murphy, Christopher K.; Kumar, Archana; Pepito, Aurora S.; Wang, Yuesheng

CORPORATE SOURCE: Cent. Sci. Technol., Syracuse Univ., Syracuse, NY, 13244, USA

SOURCE: Journal of Organic Chemistry (1993), 58(3), 718-31
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English
 OTHER SOURCE(S): CASREACT 119:138472
 AB Good yields of enantiomeric allylic alcs. can be obtained in high enantiomeric excess (ee) by combining the Sharpless-Katsuki asym. epoxidn. process (SAE) with tellurium chemical. The advantages of the tellurium process are as follows: (1) the 50% yield limitation on the allylic alc. in the Sharpless kinetic resolution (SKR) can be overcome; (2) allylic tertiary alcs. which are unsatisfactory substrates in the SKR can be obtained in high optical purity; (3) optically active secondary allylic alcs. with tertiary alkyl substituents (e.g. tert-butyl) at C-1 can be obtained in high ee; (4) optically active sterically congested cis secondary alcs. can be obtained in high ee; and (5) the nuisance of the slow SAE of some vinyl carbinols can be avoided. The key step in the reaction sequence is either a stereospecific 1,3-transposition of double bond and alc. functionalities or an inversion of the alc. configuration with concomitant deoxygenation of the epoxide function in epoxy alcs. Trans secondary allylic alcs. can be converted to cis secondary allylic alcs. by way of erythro epoxy alcs. (glycidols); threo glycidyl derivs. are converted to trans secondary allylic alcs. These transformations are accomplished by the action of telluride ion, generated in situ from the element, on a glycidyl sulfonate ester. Reduction of elemental Te is conveniently done with rongalite (HOCH₂SO₂Na) in an aqueous medium. This method is satisfactory when Te²⁻ is required to attack a primary carbon site of a glycidyl sulfonate. In cases where Te²⁻ is required to attack a secondary carbon site, reduction of the tellurium must be done with NaBH₄ or LiEt₃BH. Elemental tellurium is precipitated during the course of the reactions and can be recovered and reused.

CC 21-2 (General Organic Chemistry)
 Section cross-reference(s): 26

IT **80232-50-4P 80287-12-3P** 111321-48-3P 121401-06-7P
 121468-44-8P 121958-41-6P 131750-35-1P 131750-36-2P 131750-37-3P
 131750-38-4P 131831-36-2P 131831-37-3P 131831-38-4P 131831-39-5P
 147048-00-8P 147048-01-9P 147048-07-5P 147048-10-0P 147048-16-6P
 147127-69-3P 147127-70-6P 147127-73-9P 147127-79-5P 147127-80-8P
 147493-35-4P 200205-69-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with telluride ion)

IT 147048-17-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reduction of, with lithium aluminum hydride)

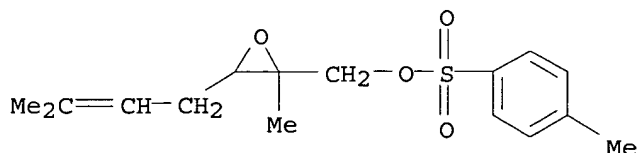
IT 62777-71-3P, (2R,3R)-2,3-Epoxygeraniol 78513-12-9P **80232-49-1P**
80299-55-4P 82188-73-6P 84039-81-6P 89194-12-7P
 97589-09-8P 107033-45-4P 107796-93-0P 114180-68-6P 114180-70-0P
 147047-99-2P 147048-15-5P 147048-20-2P 147127-72-8P 147127-74-0P
 147127-77-3P 147127-81-9P 147129-38-2P 147600-50-8P 161511-98-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and tosylation of)

IT 18448-47-0, Methyl 1-cyclohexene-1-carboxylate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of, with lithium aluminum hydride)

IT **80232-50-4P 80287-12-3P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with telluride ion)

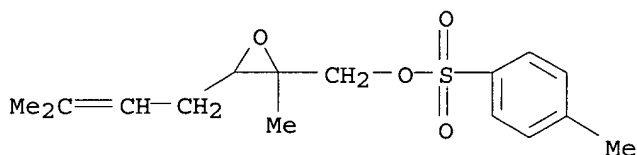
RN 80232-50-4 HCAPLUS

CN Oxiranemethanol, 2-methyl-3-(3-methyl-2-butenyl)-, 4-methylbenzenesulfonate, (2R-trans)- (9CI) (CA INDEX NAME)



RN 80287-12-3 HCAPLUS

CN Oxiranemethanol, 2-methyl-3-(3-methyl-2-butenyl)-, 4-methylbenzenesulfonate, (2S-trans)- (9CI) (CA INDEX NAME)



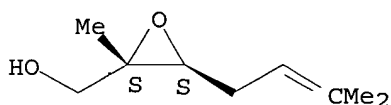
IT 80232-49-1P 80299-55-4P

RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)** (preparation and tosylation of)

RN 80232-49-1 HCAPLUS

CN Oxiranemethanol, 2-methyl-3-(3-methyl-2-butenyl)-, (2S-trans)- (9CI) (CA INDEX NAME)

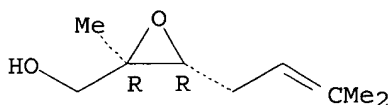
Absolute stereochemistry.



RN 80299-55-4 HCAPLUS

CN Oxiranemethanol, 2-methyl-3-(3-methyl-2-butenyl)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



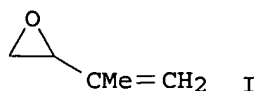
L22 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:37183 HCAPLUS

DOCUMENT NUMBER: 108:37183

TITLE: Highly regioselective addition of allylstannanes to vinyl epoxides by **Lewis** acid mediation

AUTHOR(S): Naruta, Yoshinori; Maruyama, Kazuhiro
 CORPORATE SOURCE: Fac. Sci., Kyoto Univ., Kyoto, 606, Japan
 SOURCE: Chemistry Letters (1987), (5), 963-6
 CODEN: CMLTAG; ISSN: 0366-7022
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:37183
 GI



AB Allylic trimethylstannes react with vinyl epoxides in the presence of BF₃·OEt₂ to give 1,2- or 1,4-addition products in good yield, depending on the substitution at the olefinic terminus. In either case regioselectivity is high. E.g., epoxymethylbutene I was treated with Me₂C:CHCH₂SnMe₃ to give 91% CH₂:CHCMe₂CH(CH₂OH)CMe:CH₂, which then underwent Cope rearrangement on treatment with DBU to give 100% of a 58:42 mixture of (E)- and (Z)-HOCH₂CH:CMeCH₂CH₂CH:CMe₂.

CC 23-7 (Aliphatic Compounds)
 Section cross-reference(s): 27

ST addn allylstannane vinyl epoxide regiochem; regiochem allylation vinyl epoxide; stannane allyl allylation vinyl epoxide; Lewis acid catalyst allylation regiochem; alkadienol; polyprenyl alc; alc unsatd

IT 1838-94-4 6705-51-7 6790-41-6 7437-61-8 13295-59-5
 50901-75-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (allylation of, with allylic trimethylstannanes, regiochem. of)

IT 13295-59-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (allylation of, with allylic trimethylstannanes, regiochem. of)

RN 13295-59-5 HCAPLUS

CN Oxirane, 2,2-dimethyl-3-(2-methyl-1-propenyl)- (9CI) (CA INDEX NAME)

